

```
8 9 10 11 12 13 22 23 24 25 26 27 g/chain nodes:
1 2 3 4 5 6 7 14 15 16 17 18 19 20 21 28 29 30 31 32 33 34 35 36 37 g/chain bonds:
1-2 1-5 1-6 2-3 3-4 4-7 7-8 9-14 10-17 13-35 14-15 15-16 17-18 18-19 19-20 20-21 21-22 23-28 24-31 25-32 28-29 29-30 32-33 32-34 35-36 35-37 g bonds:
8-9 8-13 9-10 10-11 11-12 12-13 22-23 22-27 23-24 24-25 25-26 26-27 ct/norm bonds:
1-2 2-3 3-4 9-14 13-35 14-15 15-16 18-19 19-20 23-28 25-32 28-29 29-30 32-34 35-37 ct bonds:
1-5 1-6 4-7 7-8 10-17 17-18 20-21 21-22 24-31 32-33 35-36 malized bonds:
8-9 8-13 9-10 10-11 11-12 12-13 22-23 22-27 23-24 24-25 25-26 26-27
```

ch level:
1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:Atom 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:CLASS
20:CLASS 21:CLASS 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:CLASS
29:CLASS 30:CLASS 31:CLASS 32:CLASS 33:CLASS 34:CLASS 35:CLASS 36:CLASS 37:CLASS

(File 'HOME' ENTERED AT 09:13:47 ON 12 AUG 2004)

FILE 'CAPLUS' ENTERED AT 09:13:59 ON 12 AUG 2004 STRUCTURE UPLOADED S L1

FILE 'REGISTRY' ENTERED AT 09:14:50 ON 12 AUG 2004 11 S L1 FULL

FILE 'CAPLUS' ENTERED AT 09:14:54 ON 12 AUG 2004

3 S L2 FULL

0 S L3 AND POLYMORPHIC?

0 S L3 AND POLYMORPH?

ictly prohibited.

E COVERS 1907 - 12 Aug 2004 VOL 141 ISS 7 E LAST UPDATED: 11 Aug 2004 (20040811/ED)

his file contains CAS Registry Numbers for easy and accurate ubstance identification.

oading C:\STNEXP4\QUERIES\861.str

STRUCTURE UPLOADED

d 11

HAS NO ANSWERS

STRUCTURE DIAGRAM IS NOT AVAILABLE ***

ucture attributes must be viewed using STN Express query preparation.

s 11 full

REG1stRY INITIATED

stance data SEARCH and crossover from CAS REGISTRY in progress... DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

L SEARCH INITIATED 09:14:50 FILE 'REGISTRY' L SCREEN SEARCH COMPLETED - 355524 TO ITERATE

.0% PROCESSED 355524 ITERATIONS

11 ANSWERS

RCH TIME: 00.00.04

11 SEA SSS FUL L1

3 L2

d 1-3 ibib abs hitstr

ANSWER 1 OF 3 CAPLUS COPYRIGHT 2004 ACS on STN

ESSION NUMBER: 1995:39068 CAPLUS

UMENT NUMBER: 123:169347

LE: preparation of phenylthiopropoxyphenyloxybutyric acid

derivatives as leukotriene antagonists

ENTOR(S): Oohashi, Mitsuo; Hori, Wataru Kyorin Seiyaku Kk, Japan ENT ASSIGNEE(S): RCE:

Jpn. Kokai Tokkyo Koho, 13 pp.

CODEN: JKXXAF

UMENT TYPE: Patent GUAGE: Japanese

ILY ACC. NUM. COUNT: 1

ENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. ____ -----------JP 06100526 -----A2 19940412 JP 1992-273717 19920917 ORITY APPLN. INFO.: JP 1992-273717

ER SOURCE(S): MARPAT 123:169347

Me A
$$CH_2$$
 CH_2 CH

Title derivs. I (A, B = CO, hydroxymethylene; E = H, OH, acetoxy; G, L = Et, acetyl, 1-hydroxyethyl, 2-hydroxyethyl, hydroxycarbonylmethyl, lower alkoxycarbonylmethyl; X = void, O, O2; R1 = H, lower alkyl; X = O, O2 and B = hydroxymethylene when A = carbonyl, E = H, and G = L = Et) or theiralkali salts, acting as strong antagonists for leukotrienes C4, D4, and E4 and useful for antiasthmatics, are prepared Thus, treating 2'-hydroxy-3'-(2-hydroxypropyl)-4'-mercaptoacetophenone (prepared in 6 steps from 3-allyl-2,4-dihydroxyacetophenone) with Et 4-[6-acetyl-3-(3bromopropoxy) -2-propylphenoxy] butyrate gave I (A = B = CO, E = H, G = 1-hydroxyethyl, L = Et, R1 = Et, X = void). 167211-60-1P 167211-72-5P 167211-78-1P 167211-82-7P 167211-90-7P 167211-91-8P 167211-92-9P 167211-93-0P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation of phenylthiopropoxyphenyloxybutyric acid derivs. as leukotriene antagonists) 167211-60-1 CAPLUS Butanoic acid, 4-[6-acetyl-3-[3-[[4-acetyl-3-hydroxy-2-(2hydroxypropyl)phenyl]thio]propoxy]-2-propylphenoxy]-, ethyl ester (9CI)

OH
$$CH_2-CH-Me$$

OH $CH_2-CH-Me$

ĽΤ

(CA INDEX NAME)

RN 167211-72-5 CAPLUS
EN Butanoic acid, 4-[6-acetyl-3-[3-[[4-acetyl-3-hydroxy-2-(3-hydroxypropyl)phenyl]thio]propoxy]-2-propylphenoxy]-, ethyl ester (9CI)
(CA INDEX NAME)

167211-78-1 CAPLUS
Butanoic acid, 4-[6-acetyl-3-[3-[(4-acetyl-3-hydroxy-2-propylphenyl)thio]propoxy]-2-(2-hydroxypropyl)phenoxy]-, ethyl ester (9CI) (CA INDEX NAME)

O AC
$$CH_2 - CH - Me$$
 AC $CH_2 - CH - Me$ AC $CH_2 - CH - Me$ AC

167211-82-7 CAPLUS

RN

CN

RN

CN

RN

CN

٩N

CΝ

Butanoic acid, 4-[6-acetyl-3-[3-[(4-acetyl-3-hydroxy-2-propylphenyl)thio]propoxy]-2-(3-hydroxypropyl)phenoxy]-, ethyl ester (9CI) (CA INDEX NAME)

O AC
$$(CH_2)_3 - S$$
 $(CH_2)_3 - OH$ AC $(CH_2)_3 - OH$ AC

167211-90-7 CAPLUS

Butanoic acid, 4-[6-acetyl-3-[3-[[4-acetyl-3-hydroxy-2-(2-oxopropyl)phenyl]thio]propoxy]-2-propylphenoxy]-, ethyl ester (9CI) (CA INDEX NAME)

167211-91-8 CAPLUS

Butanoic acid, 4-[6-acetyl-3-[3-[(4-acetyl-3-hydroxy-2-propylphenyl)thio]propoxy]-2-propylphenoxy]-, methyl ester (9CI) (CFINDEX NAME)

167211-92-9 CAPLUS

Butanoic acid, 4-[3-[3-[(4-acetyl-3-hydroxy-2-propylphenyl)thio]propoxy]-6-(chloroacetyl)-2-propylphenoxy]-, methyl ester (9CI) (CA INDEX NAME)

167211-93-0 CAPLUS

Butanoic acid, 4-[3-[3-[(4-acetyl-3-hydroxy-2-propylphenyl)thio]propoxy]-6-[(acetyloxy)acetyl]-2-propylphenoxy]-, methyl ester (9CI) (CA INDEX NAME)

$$0 - C = 0$$
 $0 - C = 0$
 $0 -$

ANSWER 2 OF 3 CAPLUS COPYRIGHT 2004 ACS on STN

SION NUMBER: 1990:138760 CAPLUS

MENT NUMBER: 112:138760

:: Preparation of phenoxyalkylcarboxylic acid derivatives

as antiallergic agents

TOR(S): Ohashi, Mitsuo; Awano, Katsuya; Tanaka, Toshio;

Kimura, Tetsuya

T ASSIGNEE(S): Kyorin Pharmaceutical Co., Ltd., Japan

Eur. Pat. Appl., 32 pp.

CODEN: EPXXDW

ENT TYPE: Patent IAGE: English

Y ACC. NUM. COUNT:

T INFORMATION:

'E:

PAT	TENT NO.			KIND	DATE	APPLICATION NO.	DATE
	332109 332109			A1 B1	19890913 19911204	EP 1989-103897	19890306
	R: BE,	CH,	DE,	ES, FR	, GB, IT,	LI, NL, SE	
JΡ	02001459	•		A2	19900105	JP 1989-38912	19890218
JΡ	07116125	5		B4	19951213		
US	4985585	•		A	19910115	US 1989-313900	19890223
ΑU	8930884			A1	19890907	AU 1989-30884	19890301
ΑU	617439			B2	19911128		
CA	1331763			A1	19940830	CA 1989-592555	19890302
HU	50112			A2	19891228	HU 1989-1039	19890303
HU	204030			В	19911128		
HU	208418			В	19931028	HU 1991-2410	19890303
HU	208524			В	19931129	HU 1991-2411	19890303
ES	2045219			Т3	19940116	ES 1989-103897	19890306
CN	1036560			A	19891025	CN 1989-101301	19890307
CN	1022407			В	19931013		
ITY	APPLN.	INFO	. :			JP 1988-53374	19880307
						HU 1989-1039	19890303
SC	URCE(S):			MARPAT	112:13876	0	

MeCO
$$X^1 (CH_2)_m X^2$$
 $COMe$
HO Pr Pr O(CH₂)_nCO₂R¹ I

COMe MeCO
$$\rightarrow$$
 S (CH₂) 3Br \rightarrow O (CH₂) 3CO₂Et II HO Pr III

The title compds. (I; R1 = H, Me, Et; X1, X2 = O, S, SO, SO2; X1 = X2 # O; m = 2-5; n = 3-8), useful as antiallergic agents, are prepared A mixture of phenoxybutyrate II, bromopropyl thioether III, KI, and K2CO3 in Me2CO was refluxed to give 72.4% I (R1 = Et, X1 = S, X2 = O, m = n = 3). I showed 66.7-96.2% inhibition of leukotriene D4-induced pronchoconstriction at 50 mg/kg p.o. in guinea pigs. Addnl. 70 I were also prepared

125961-80-0P 125961-81-1P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of, as antiallergic agent)

125961-80-0 CAPLUS

Butanoic acid, 4-[6-acetyl-3-[3-[(4-acetyl-3-hydroxy-2-

propylphenyl)sulfinyl]propoxy]-2-propylphenoxy]-, ethyl ester (9CI) (CFINDEX NAME)

125961-81-1 CAPLUS

Butanoic acid, 4-[6-acetyl-3-[3-[(4-acetyl-3-hydroxy-2propylphenyl)sulfonyl]propoxy]-2-propylphenoxy]-, ethyl ester (9CI) (CA INDEX NAME)

ANSWER 3 OF 3 CAPLUS COPYRIGHT 2004 ACS on STN

SION NUMBER: 1983:575604 CAPLUS

ENT NUMBER: 99:175604

Anti-SRS-A carboxylic acid derivatives and pharmaceutical formulations containing them

TOR(S): Bantick, John Raymond
T ASSIGNEE(S): Fisons Ltd., UK

Eur. Pat. Appl., 67 pp.

CODEN: EPXXDW

ENT TYPE: Patent AGE: English

Ε:

T INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 79637	A1	19830525	EP 1982-201368	19821101
EP 79637	B1	19870128		
R: AT, BE, CH,	DE, FR	, GB, IT, L	I, LU, NL, SE	
US 4474788	Α	19841002	US 1982-438163	19821101
AT 25251	E	19870215	AT 1982-201368	19821101
JP 58090557	A2	19830530	JP 1982-196883	19821111
ITY APPLN. INFO.:			GB 1981-34186	19811112
			EP 1982-201368	19821101

$$R^{5}$$
 R^{4}
 R^{3}
 R^{3

Anti-allergy (no data) bicyclic compds. I [R, R1 = H, alkyl; RR1 = bond; R2 = CO2H, carboxyalkyl; R3 = substituted OH, SH, NH2; R4, R5 = H, halogen, (un)substituted OH, NH2, alkyl, acyl; X = S, O, NR6 (R6 = H, alkyl)] were prepared Thus, 3,2,4-Pr(HO)2C6H2Ac reacted with 4,2,3-AcPr(H2N)C6H2S(CH2)3Br to give phenol II, which cyclized with EtO2CCO2Et to give quinoline III [R7 = Et, R8R9 = CH:C(CO2Et)]. The latter compound gave III (R7 = H, R8 = Me, R9 = H) on hydrolysis. 87472-34-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and hydrolysis of)

87472-34-2 CAPLUS

4H-1-Benzopyran-2-propanoic acid, 7-[3-[(4-acetyl-3-hydroxy-2-propylphenyl)thio]propoxy]-4-oxo-8-propyl-, ethyl ester (9CI) (CA INDEX NAME)